

# **Department of Energy**

Washington, DC 20585

November 15, 2000

Mr. Paul W. Kruger
Assistant Manager for Science and Technology
U.S. Department of Energy
Richland Operations Office
825 Jadwin Avenue
Richland, Washington 99352

Dear Mr. Kruger:

For fiscal year 2000, the Pacific Northwest National Laboratory's (PNNL) overall performance on Office of Science (OSC) science and technology programs is rated as Outstanding. This rating relates to the scale that includes Unsatisfactory, Marginal, Good, Excellent, and Outstanding. It is a weighted average of performance evaluations provided by each OSC program office, with the budget for Pacific Northwest from each office as the weighting factor. This summary rating combines overall performance evaluations for program areas supported by the OSC offices of Basic Energy Sciences, Biological and Environmental Research, Advanced Scientific Computing Research, and Fusion Energy Sciences.

Although the overall rating is Outstanding, several concerns have been expressed by the OSC Program Managers. For the second year in a row, the Office of Basic Energy Sciences (BES) expressed significant concerns over the laboratory's ability to balance the coupling between BES' Metal and Ceramic Sciences program and technology programs funded by other applied program offices of DOE and the Electric Power Research Institute. They state that the problem is manifest to such an extent "that there is concern that the climate at PNNL may not be the most conducive to inquiry driven fundamental science, with a maximum reasonable opportunity to exploit innovative and creative cutting edge or frontier research. Such research may be viewed at PNNL as not consistent with the preconceived milestones of these technology programs." Also, the Office of Biological and Environmental Research observes that PNNL has a significant scientific leadership gap in Life Sciences research. Attention is needed to resolve these problems. I look forward to working on them with you.

Enclosure 1 summarizes the overall OSC weighted average ratings by each goal. Enclosure 2 presents the individual OSC Programs' ratings of the laboratory's performance for each of the performance evaluation factors. Also enclosed are full narrative evaluations from each program area.

Sincerely,

mildred J. Dresselhaus

Mildred S. Dresselhaus Director Office of Science

**Enclosures** 

# **Enclosure 1:**

# OFFICE OF SCIENCE PACIFIC NORTHWEST NATIONAL LABORATORY EVALUATION FY 2000 OSC WEIGHTED AVERAGE RATINGS BY GOAL:

OVERALL CONSOLIDATED RATING: OUTSTANDING

Weighted Average Score:

3.57

Goal: 01

Quality of Science & Technology

Consolidated Rating:

**OUTSTANDING** 

Weighted Average Score:

3.54

Goal: 02

Relevance to DOE Missions or National Needs

Consolidated Rating:

**OUTSTANDING** 

Weighted Average Score:

3.56

Goal: 03

Success in Constructing and Operating Research Facilities

Consolidated Rating:

**OUTSTANDING** 

Weighted Average Score:

3.90

Goal: 04

Effectiveness and Efficiency of Research Program Management

Consolidated Rating:

**OUTSTANDING** 

Weighted Average Score:

3.52

# PACIFIC NORTHWEST NATIONAL LABORATORY FY 2000 RATINGS OF EACH GOAL BY EACH OSC PROGRAM

G = Good; E = Excellent; O = Outstanding

	Goal 1: Quality	Goal 2: Relevance	Goal 3: Facilities	Goal 4: Program Mgt.	Overall Program Rating	Overall ER Weighted Average
BES	3.40 - E	3.20 - E	N/A	3.00 - E	3.20 - E	
BER	3.40 - E	3.50 - O	3.90 - O	3.63 - O	3.61 - 0	
ASCR	3.77 - O	3.83 - O	3.90 - O	3.64 - O	3.79 - 0	
Fusion	3.60 - O	3.70 - 0	N/A	3.80 - O	3.70 - O	
OVERALL	3.54 - O	3.56 - O	3.70 - O	3.70 - O		3.57 - O

#### **Aristides Patrinos**

Pacific Northwest National Laboratory Performance Appraisal FY 2000 by the Environmental Sciences Division, SC-74

Reviewer Elwood

Goal 01: Quality of Science & Technology -

Score: 3.4

Overall, PNNL's science and technology is of high merit. Specifically, the science and management of the Atmospheric Radiation Measurement (ARM) program has been of superior quality. PNNL has responsibility for two roles in ARM: engineering and design and the overall coordination of the ARM infrastructure across the ARM elements. The development of algorithms for new science products has been exceptional. Additionally, the Science Applications Group has made tremendous strides in building partnerships with the science team. Research efforts are well recognized, with respected, original scientific contributions being made to the field. For example, research conducted at and near the ARM site in Barrow, Alaska, is contributing to the understanding of the complex relation between surface characteristics such as albedo, and the type and physical character of the clouds in the region. PNNL is a highly recognized institution in the global change scientific community.

A number of projects at PNNL have made state-of-the-science contributions to DOE's Atmospheric Chemistry Program (ACP) and to DOE's Environmental Meteorology Program (EMP). For example, (1) Five peer-reviewed publications have resulted from the project entitled "A Quantitative Assessment of the Role of Heterogeneous Chemistry and Mixing on NOy in the Nightime Atmospheric Boundary Layer" and uncertainties associated with simulations of nighttime chemistry and aerosols in atmospheric chemistry/transport models have been reduced. (2) Three peer-reviewed publications have resulted from the project entitled "Nucleation of Tropospheric Aerosols: A Joint Laboratory and Theoretical Study of Multicomponent Systems" and a new theoretical approach has been developed to treat homogeneous vapor-phase nucleation. (3) Three peer-reviewed publications have resulted from the project entitled "The Dependence of urban Scale Oxidant Chemistry on Boundary-Layer Processes and Regional-Scale Transport."

PNNL has a solid technical base that impacts a number of fields, from genomics to bioremediation. They have a strong environmental microbiology group, and efforts to bring greater leadership to this group should continue. They consistently publish high quality research in peer-reviewed publications.

PNNL's contribution to bioremediation and the NABIR program is impressive. Many researchers contribute to the scientific success of NABIR, consistently performing well in competitions for funding. The researchers provide both exceptional research results and coordinate well with other researchers in the NABIR program by collaborating on research projects and providing specialized expertise.

Scientists within the Environmental Molecular Sciences Laboratory (EMSL) at PNNL are recognized as being at the leading edge of structural biology research using mass spectrometry and NMR, oxide chemistry, basic materials science and nanoscience, and computational chemistry associated with environmental issues. The results of research by EMSL scientists have been published and featured in a wide variety of prestigious journals within the past year.

Reviewer Elwood

Goal 02: Relevance to DOE Mission and National Needs

The ARM program is attacking the uncertainty in predicting climate change that addresses a major DOE mission and national issue. The development and operation of the ARM sites responds to the climate prediction problem by providing the facilities needed by the teams of principal investigators in ARM. PNNL leads the ARM Program's extensive interaction with related non-DOE research, especially with regard to cooperation with NASA, NOAA, and other U.S. Government research organizations. PNNL also leads in coordination with international efforts such as the recent Nauru99 efforts, which involved Japanese assets and researchers. PNNL should keep the ARM web page up to date with scientific success stories and accomplishments.

All of the atmospheric science projects at PNNL are quite relevant to both national and agency needs to understand the processes governing the distribution and fate of energy-related pollutants.

PNNL's current programs contribute to NABIR, EMSP and terrestrial carbon sequestration. Work in proteomics will have broad impact across mission areas.

PNNL researchers involved with the integrated assessment modeling effort and the Technology Strategy Project not only connect well to DOE missions but also in some sense anticipate DOE issues. For example, the Technology Strategy Project has developed themes and provided a context that help DOE plan for long-term DOE research programs. Senior researchers at PNNL have notably contributed to carbon sequestration roadmapping exercises as well as to a high-level analysis of DOE's energy research portfolio.

#### **Aristides Patrinos**

PNNL has also contributed very high quality staffing for the International Panel on Climate Change. That expertise has resulted in further staffing for internal assessment activities for the U.S. Global Change Research Program.

Office of Science (SC) research within PNNL is well focused on DOE needs, and most research funded by DOE at PNNL is within the DOE mission areas. DOE-funded facilities and capabilities should be primarily used to support DOE's mission areas.

Reviewer Elwood

Goal 03: Success in Constructing and Operating Research Facilities

Score: 3.9

The ARM sites are recognized facilities for atmospheric science.

The Research Aircraft Facility at PNNL is exceptionally well managed. Of particular note is the role of management during operational crises, in protecting people (first and foremost) and in quickly restoring operational capability in support of research scientists.

Now in its third year of operation, the William R. Wilcy Environmental Molecular Sciences Laboratory (EMSL) continues to be well managed and to attract users from a wide variety of disciplines. The annual user meeting was quite successful, informative, and innovative in format. As of the end of the third quarter of FY00, the total number of users had increased substantially over that during the same time period in FY99. Participation from the academic community and from non-visiting users continued to remain quite high. Based on the annual user survey, user satisfaction also remained high. Research conducted by EMSL scientists and by EMSL users needs to remain focused on DOE's environmental needs.

Reviewer Elwood

Goal 04: Effectiveness and Efficiency of Research Program Management

Score: 3.7

The management for the newly created Engineering Team has provided excellent leadership in developing systems and algorithms that respond to ARM's scientific requirements. The ARM Project Manager has provided excellent overall coordination among the ARM management elements. Communication of scientific results has been excellent, and the Chief Scientist has represented the science objectives and progress to a wide assortment of groups both nationally and internationally. Overall, PNNL management of ARM projects is outstanding. PNNL has had tremendous success in addressing various issues such as budget impacts stemming from instrumentation development, deployment and operation. Greater effort is needed to keep all relevant HQ program managers informed of ARM developments.

The Lead Scientist for DOE's Atmospheric Sciences program has done an outstanding job in marshalling, organizing, and implementing community resources in support of the Vertical Transport and Mixing Experiment (VTMX). The result is an exceptionally well-planned and coordinated activity, within budget, that is expected to be both an operational and scientific success.

Overall, research management is satisfactory. Technical results are communicated well.

PNNL has efficiently and effectively operated the EMSL as a National Scientific User Facility. Although funding for operations was not conducive to growth, the EMSL was operated with maximum efficiency. EMSL management responds quickly and thoroughly to Headquarters requests for information and/or data, and they keep Headquarters managers well informed of EMSL activities and issues.

Pacific Northwest National Laboratory FY 2000 Appraisal by the Life Sciences Division SC-72

Reviewer Frazier

Goal 01: Quality of Science and Technology

SCORE: 3.6

PNNL has relatively few Life Sciences research projects. The projects span the areas of proteomics, low dose radiation research and structural biology. The largest of the projects is in proteomics. This effort was reviewed twice during FY 00 by groups of external experts and was found to be of exceptionally high scientific quality. The other Life Sciences projects at PNNL are making good progress and have the potential to make substantial contributions to their fields.

Reviewer Frazier

Goal 02: Relevance to DOE Mission and National Needs

SCORE: 3.7

PNNL's Life Science research projects are highly relevant to DOE and National needs.

Reviewer Frazier

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#### **Aristides Patrinos**

Goal 03: Success in Constructing and Operating Research Facilities

Not applicable

Reviewer Frazier

Goal 04: Effectiveness and Efficiency of Research Program Management

SCORE: 2.0

PNNL's Life Sciences research efforts are very responsive to DOE needs and concerns. These projects are part of larger DOE and National efforts requiring close coordination, monitoring of progress and adherence to project goals. In spite of the success of these specific projects, PNNL has a significant scientific leadership gap in Life Sciences research. This leadership gap has, no doubt, been a factor in PNNL's relative lack of success in obtaining funds for new Life Sciences research. Efforts are underway to correct this deficiency.

PNNL Appraisal FY 2000 by the Medical Sciences Division, SC-73

Reviewer Viola

Goal 01: Quality of Science & Technology

Score: 3.5

Research projects in both Medical Applications/Measurement Science and in Structural Biology are considered outstanding. The nuclear magnetic resonance (NMR) microscopy and NMR and mass spectrometry projects have achieved considerable success in advancing the capabilities of those techniques. The research has provided a strong base of instrumentation for the emerging field of proteomics.

Reviewer Viola

Goal 02: Relevance to DOE Mission and National Needs

Score: 3.5

The projects in Medical Applications/Measurement Science and in Structural Biology are relevant to DOE mission responsibilities in the biological sciences. The new techniques allow both imaging of the chemical contents of microscopic regions of biological tissues, and determination of the detailed chemical composition of these samples, a first step in addressing many research areas in the life sciences in which the Department has a strong interest, including bioremediation, the carbon cycle, and DNA damage repair mechanisms.

Reviewer Viola

Goal 03: Success in Constructing and Operating Research Facilities:

Not applicable.

Reviewer Viola

Goal 04: Effectiveness and Efficiency of Research Program Management

Score: 3.3

The projects in Medical Applications/Measurement Science and in Structural Biology are well managed. The relatively modest funding has resulted in high productivity. Communications from the Laboratory to DOE are excellent, with prompt notification of major developments, such as prominent publications.

### Patricia M. Dehmer

Office of Basic Energy Sciences

FY 2000 Evaluation of Science and Technology Performance for Pacific Northwest National Laboratory

Reviewer Dehmer

Goal 01: Quality of Science and Technology

Rating: 3.4 (Excellent)

The fundamental research supported by the Chemical Sciences program at PNNL is directly related to the environmental mission of the agency including those specifically relevant to the Hanford site. The research performed through this program is directed towards interfacial science and includes, amongst others, fundamental studies of the interaction of liquid-interfacial chemistry, energetic processes in condensed phases, kinetics of surface reactions, supercritical fluids, analysis, as well as theoretical efforts related to interfaces. As judged by external peer reviews, the quality of the staff and the science performed is excellent. Reviewers have made comments that some of the work at PNNL will require modification to textbooks and that other aspects of the program are truly "world-class." The program is technically very relevant and of very high quality.

The BES Geosciences program at PNNL supports excellent research on basic theoretical and experimental surface geochemistry. The program underpins technologies important for the Department's environmental missions. A new project was funded in FY 2000 as a top candidate identified in the Complex and Collective Phenomena Initiative.

The quality of science for the Metal and Ceramic Science program at Pacific Northwest National Laboratory (PNNL) is excellent overall, and outstanding in some areas. This judgement is based on the DOE managed on-site peer review in June 1999, a peer review managed by PNNL management in June 2000, site visits, and recent achievements such as the following two items:

The first is work under Dr. W. J. Weber concerning the durability of gadolinium zirconate as a radioactive waste host has received international acclaim. Using heavy-ion irradiation, advance characterization techniques, and computer simulation methods, Weber and his partners have discovered that highly durable gadolinium zirconate can lock plutonium into its structure while remaining extremely resistant to radiation damage.

The second is the discovery by PNNL researchers that high quality, close-packed and oriented nanostructure materials based on self-assembled monolayers of functional molecules on ordered nanoporous can be produced and efficiently assembled. Time dependent high-resolution magnetic resonance experiments suggested that the properties of the monolayers, including the cross-link density and the flexibility of the functional molecules in the porous media, are related to the molecular chain length and to the pore size and shape. Two- or three-dimensional binding sites can also be constructed on the monolayer so that the shape and geometry of these molecular binding sites match those of the target molecules or species. Furthermore, using a molecular directed synthesis approach, specific functional molecules can be delivered to a pre-determined site on the monolayer, forming spatially organized molecular monolayers in which the distribution of the functional groups and molecules are tightly controlled. These results have potential for breakthrough technologies in environmental remediation, energy storage, catalytic chemistry, transportation, microelectronic devices, and controlled- and time-release reactions for biomedicine and agriculture.

Reviewer Dehmer

Goal 02: Relevance to DOE Mission or National Needs

Rating: 3.2 (Excellent)

A major technical concern of the Department -- and a mission that is a critical national need -- is the required 'clean-up' of facilities. Both the Chemical Sciences and Geosciences supported programs at PNNL are providing the theoretical foundation and experimental verification for understanding the fundamentals of how metals and other contaminants bind to mineral surfaces, and therefore, how they can be removed. These programs have built the foundation for a number of successful applications to the Office of Environmental Management in the Environmental Management Science Program.

The coupling between the Metal and Ceramic Sciences program with technology programs at PNNL such as those funded by the DOE Office of Energy Efficiency and Renewable Energy and the Office of Fusion Energy Sciences, as well as one funded by the Electric Power Research Institute, is extremely tight. It is to such an extent that there is concern that the climate at PNNL may not be the most conducive to inquiry driven fundamental science, with a maximum reasonable opportunity to exploit innovative and creative cutting edge or frontier research. Such research may be viewed at PNNL as not consistent with the preconceived milestones of these technology programs. The need for an appropriate balance is discussed under Goal 04.

Reviewer Dehmer

Goal 03: Success in Constructing and Operating Research Facilities:

Not Applicable

#### Patricia M. Dehmer

Reviewer Dehmer

Goal 04: Effective and Efficient Program Management

Rating: 3.0 (Excellent)

With respect to the Chemical Sciences program, laboratory management has been quite responsive to program needs. However, there have been concerns about the fractured management of the subprograms with different parts reporting to different management organizations. The laboratory is taking action to consolidate the subprograms under one management structure.

As indicated above under Goal 02 for the Metal and Ceramic Sciences program, there is a concern about the excessive coupling between the work supported at PNNL and the needs of the co-sited applied programs to comply with their milestones. This concern was previously noted by a reviewer at the on-site peer review of June 1999: "The program makes effective coupling with technology oriented programs and are able to leverage the support from Basic Energy Sciences. However, this close connection also carries some risk which the management should constantly address. The research must be of intrinsic value to basic science and would be justified and conducted in the absence of the associated applied activities." During the past year, PNNL has designated a new program coordinator for the BES/Materials Sciences and Engineering program.

#### N. Anne Davies

Associate Director, Office of Fusion Energy Summary:

The Pacific Northwest National Laboratory's (PNNL) fusion-related efforts are of modest size. Nevertheless, the program continues to be focussed on major tasks of the Office of Fusion Energy Sciences' Advanced Materials Program. They have demonstrated leadership in management of US/Japan collaborations on fusion materials. They remain at the forefront of research on silicon carbide composite materials and have made important contributions to the vanadium alloy, ferritic steel, and modeling materials program elements. The overall quality of PNNL work on fusion materials continues to be outstanding.

OVERALL RATING AND SCORE: Score: 3.7 - Outstanding

Reviewer Berk:

Goal 1: Quality of Science

SCORE = 3.6

PNNL continues to contribute research of the highest quality in the program to develop a knowledge base on fusion materials. They provide cutting edge research on silicon carbide composite materials, and also provide important contributions to the vanadium alloy, ferritic steel, and modeling program elements. Steady progress is being made on all Advanced Materials Program tasks. The overall quality of work continues to be outstanding.

Goal 2: Relevance to DOE Missions or National Needs

Reviewer Berk:

SCORE = 3.7

The Advanced Materials Program is a key element of the US Fusion Energy Sciences Program. PNNL continues to focus efforts on the most important tasks of the Advanced Materials Program. They are responsive to DOE and fusion community input in setting the direction of their work.

Goal 3: Success in Construction and Operation of Facilities

Reviewer Berk: Not Applicable

Goal 4: Effective and Efficient Research Program Management

Reviewer Berk:

SCORE = 3.8

PNNL has taken responsibility in leading the Advanced Materials Program for SiC/SiC Composite materials and in managing the US/Japan collaboration on fusion materials. PNNL has also shared with DOE the task of conducting programmatic discussions and planning within the Advanced Materials Program Leaders Group. They continue to perform in superior manner in these roles. PNNL made important contributions to the development of a roadmap for the Advanced Materials Program. They also shared leadership of a planning activity for a possible program redirection that would put greater emphasis on the theory/modeling of materials behavior, and integration of the theory and modeling with the experimental program.

**Ed Oliver** 

Laboratory Technology Research Subprogram Reviewers: Sam Barish/Walter Polansky

Reviewer Barish

Goal 01: Quality of Science and Technology -

Rating: Outstanding 3.7

Pacific Northwest National Laboratory continues to study very important scientific questions and produce high-quality scientific results. An example is a project designed to gain a fundamental understanding of how interfaces affect the dielectric and ferroelectric properties of barium strontium titanite thin films, and to use such knowledge to improve the design and processing of BST thin film-based devices. The objective of another project is to understand the collective and complex nonlinear dynamical behavior of crystalline materials by merging a set of highly sophisticated experiments, using computer aided, massive numerical analyses, and experimental data. The project will have an impact on future computational and experimental advances in dislocation theory and will improve prospects for predictive alloy properties control.

A PNNL Principal Investigator of an LTR project received significant recognition during FY 2000. Dr. Richard Smith was named the Battelle Inventor of the Year. Dr. Smith is an internationally recognized expert in mass spectrometry and separation techniques. He was the PI of an LTR project, entitled 'High Sensitivity Electrospray Ion Source Development.'

This year, two PNNL multi-year projects were subjected to a mid-program peer review. The results of each review demonstrated that each project had made good scientific progress. Accordingly, both projects will be continued to completion as scheduled.

Reviewer: Barish

Goal 02: Relevance to DOE Mission and National Needs

Rating: Outstanding 3.8

PNNL LTR projects strongly support DOE missions and national needs. These projects include development and validation of a computational approach for modeling and simulation of ultra-thin interfaces of Silicon with high-dielectric-constant materials; development of a three-dimensional heat transfer finite element code that is capable of modeling heat transfer for optically thin and/or thick materials, such as non-gray materials like glass; and development and optimization of a core-wire direct casting technology for the production of titanium wire and rod products.

Reviewer: Barish

Goal 03: Success in Constructing and Operating Research Facilities

Rating: Does Not Apply

Reviewer: Barish

Goal 04: Effectiveness and Efficiency of Research Program Management -

Rating: Outstanding 3.5

PNNL responded well to the FY 2000 initiative for Rapid Access Projects. All three of their proposals for Technical Assistance Projects were funded. Two of their four proposals for small CRADAs were funded. All funded projects were of good scientific/technical quality.

The PNNL LTR office has been responsive to the requests from DOE headquarters concerning conduct of the LTR program.

Mathematical, Information, and Computational Sciences Subprogram

Reviewer: Mary Anne Scott

Reviewer: Scott

Goal 01: Quality of Science and Technology-

Rating: Outstanding 3.9

PNNL is involved in several projects that were initiated under the DOE2000 program. Specifically, they support several R&D projects-electronic notebooks, collaborative session management, and collaboratory interoperability framework and have a project that is part of the ACTS Toolkit-Global Arrays. All these efforts involve integrated activities across multiple laboratories and organizations. Their work is outstanding and the contribution to the MICS program in their respective areas is very valuable. Their commitment to the concept and implementation of collaborative technology is clear by virtue of applying their experience to the EMSL facility-it is a core part of the facility with the remote operation of the NMR instruments becoming more and more popular for users. Their work is excellent and their contribution to the enabling tools for collaboratories is outstanding. They are well recognized in the field of collaborative technologies. After organizing and conducting a successful workshop on collaborative problem solving environments that brought together researchers from a wide range of disciplines supported by a number of funding sources, there have been followups among attendees who agreed to work together. A report was prepared; a web site focused on this community was organized and a technical session is being organized as part of

#### **Ed Oliver**

the Software Technology Track for the HICSS-34 conference scheduled in early 2001.

All these projects were reviewed this past year and the reviewers provided very favorable comments.

Reviewer: Scott

Goal 02: Relevance to DOE Mission and National Needs -

Rating: Outstanding 3.9

Partnering across science and technology programs is an important element to the structure and goals of the MICS program that supports these projects. PNNL fully supports this partnering and provides effective championing of this goal within the broader community. Under the electronic notebook, the goal is to design a modular, extensible notebook architecture and define a base set of notebook functionality. The acceptance and value of the work is attested to by the large number of users who have adopted the early reference implementation of the notebook for use and by the interest of the Collaborative Electronic Notebook Systems Consortium, with their efforts to create and expand the markets for scientific laboratory software.

Reviewer: Scott

Goal 03: Success in Constructing and Operating Research Facilities

Rating: Outstanding 3.9

While the work supported by the DOE 2000 projects does not include operation, the influence of the direction of the projects has been very influential in the operations and the tools developed there. Specifically, the CORE2000 toolkit developed as a DOE2000 project, is a key element to remote operation of the Virtual NMR Facility. At the last review of projects proposed for the NMR instruments, a large percent indicated that they plan to rely on only remote operation. A number of others plan to visit for the first operation, then rely on remote operations.

Reviewer: Scott

Goal 04: Effectiveness and Efficiency of Research Program Management

Rating: Outstanding 3.9

These projects involve planning across multiple organizations. This is done well and appropriate milestones have been met. From a management perspective, they have shown leadership in promoting a cohesive collaboration environment across the R&D projects and the pilot collaboratories. Their activities are a positive contribution and they have also made important contacts in the research community outside of DOE who are pursuing R&D in the same or similar areas.